

2,2,2-Trifluoroethanol  
75-89-8 | DTXSID0021751

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

## Model Results

**Predicted value:** 3.51e-01

**Global applicability domain:** Inside

**Local applicability domain index:** 5.43e-01

**Confidence level:** 7.16e-01

## Nearest Neighbors from the Training Set

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2,2,2-Trifluoroethanol

**Measured:** 0.41

**Predicted:** 3.51e-01

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Ethanamine, 2,2,2-trifluoro-

**Measured:** 0.24

**Predicted:** 3.15e-01

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1,1,1-Trifluoro-2-propanol

**Measured:** 0.71

**Predicted:** 7.68e-01

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2-Propanol, 1,3-difluoro-

**Measured:** -0.360

**Predicted:** -0.0748

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Methyl acetate

**Measured:** 0.18

**Predicted:** 1.23e-01